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COMPARISON OF QUALITATIVE CRITERIA IN DECISION ON NUMBER OF COLLAGEN FIBRE FAMILIES IN SOFT TISSUES

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Abstract: *In biomechanics of soft tissues, especially of arteries, collagen fibres play an important role. They are arranged in different directions creating thus fibre families with a main direction and a certain dispersion. The number of this families in different arteries and their layers is still questionable although many researchers presume existence of two helical fibre families. We have analysed histograms published in three papers and shown that the presumption on two fibre families may be misleading; in some cases, unimodal or isotropic distributions gave a better quality of the fit than the bimodal distribution. Although we expected that information criteria could strengthen our objections against the generally applied assumption on two fibre families in arterial wall, this was not confirmed and the preferred approximation function was always the same for both of the compared criteria (Akaike information criterion and coefficient of determination R^2).*

Keywords: Akaike information criterion, Coefficient of determination R^2, Collagen fibres, Arterial wall.

1. Introduction

In biomechanics of many soft tissues, collagen fibres have an important role in their mechanical response. In arteries, collagen is arranged in fibre families and the question about the number of collagen fibre families in individual layers of arterial wall is still not answered. Many authors – e.g. (Holzapfel et al., 2000) – assume two fibre families without histological substantiation while, on the contrary, some published histograms of fibre directions show only one fibre family (Gaul et al., 2017, Polzer et al., 2015). The number of fibre families and fibre dispersion is determined from the histograms mostly by using von Mises distribution (Gasser et al., 2006), which can be unimodal, bimodal, or multimodal. However, some histograms do not show a unique number of fibre families; the applied approximation may then have a significant impact on the mechanical response of the tissue and should be chosen rigorously. In this paper, Akaike information criterion (AIC) and coefficient of determination R^2 are used for comparison of goodness of fit of different approximations of experimental data on collagen fibres distribution in soft tissues.

2. Methods

Experimental histological data on distribution of collagen fibres in arterial wall published in three different papers were used. Mathematical fundamentals of both compared criteria are presented in this paragraph.

2.1. Coefficient of determination R^2

Coefficient of determination R^2 denotes goodness of fit of a regression model in statistics. It reaches values up to 1 representing a perfect fit while negative values mean the fit is even worse than fitting with a constant. Then it makes sense to add a constant to the chosen function (Barten, 1987). However, R^2 has one major drawback – it does not prevent overfitting, which means a model has better R^2 due to its higher number of parameters. Extremely, a polynomial of n^{th} order must give $R^2 = 1$ for any function given by not more than (n+1) observations (experimental points). R^2 is defined by (Barten, 1987):

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} \tag{1}$$

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where SS_{res} is a sum of squares of residuals and SS_{tot} is a total sum of squares.

2.2. Akaike information criterion

Generally, information criteria prevent overfitting through penalization of number of parameters. In our case AIC is used to compare suitability of bimodal and unimodal distributions. Originally it was developed for maximum likelihood estimation (MLE) and was defined by (Akaike, 1974) as follows:

$$\mathrm{AIC} = -2 \cdot \log f(x) + 2K, \tag{2}$$

where $f(x)$ is a likelihood function and K is its number of estimated parameters. However, in this study an alternative form of AIC is used based on the least square method (Glatting et al., 2007):

$$\mathrm{AIC} = n \cdot \ln \frac{SS}{n} + 2(K+1), \tag{3}$$

where n is number of observations, K is number of estimated parameters and SS is total sum of squares.

AIC is a comparative criterion, applicable only for comparison of more than one function to decide on the best approximation of the data – the lower is the AIC value (in mathematical sense, i.e. also more negative), the better is the fit.

The following example illustrates differences between both criteria and advantages of penalization of the number of used parameters. Fictitious experimental data (see Fig. 1) may be fitted with polynomial functions of different orders, and if we compare polynomials of 1st and 5th order, the latter gives better R^2 but by virtue of more parameters used. In contrast, the AIC penalizes the number of used parameters and shows a linear function describes the data better (see Tab. 1).

Tab. 1: Comparison between R^2 and AIC for the model example.

Function	Number of parameters	R^2	AIC
Linear (1st order polynomial)	2	0.9476	−2.6443
Polynomial (5th order polynomial)	6	0.9601	2.3529

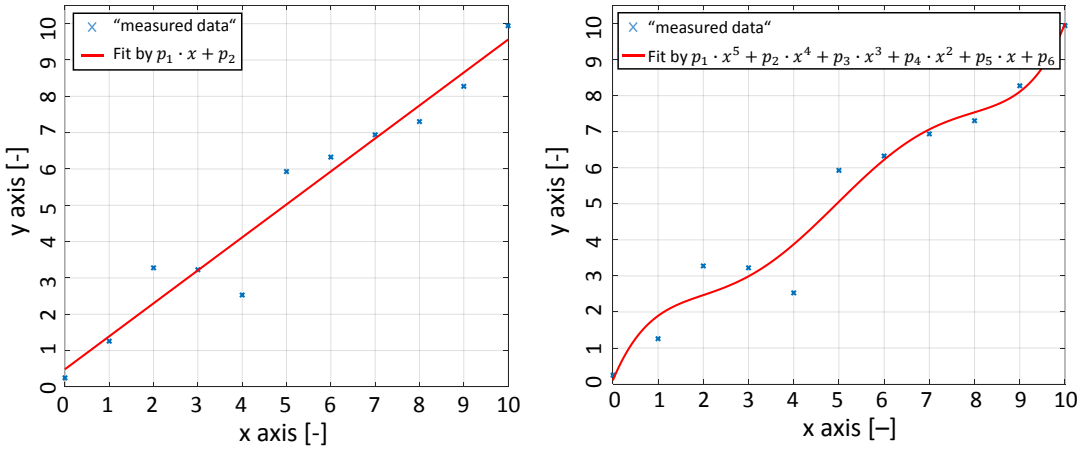

Fig. 1: Comparison of 1st and 5th order polynomial functions.

2.3. Mathematical description of distributions

For mathematical description of collagen fibres, von Mises distribution is used. It is a circular distribution and represents an equivalent of normal distribution in linear statistics. Since two vectors with opposite orientation define the same direction of fibre, π-periodic von Mises distribution is used. Unimodal von Mises probability distribution function (PDF) is defined as follows (Wang et al., 2012):

$$\rho(\phi) = \frac{1}{\pi I_0(b)} \mathrm{e}^{b \cos(2\cdot(\phi-\mu))}, \tag{4}$$

where $b \in \langle 0; \infty)$ is a concentration parameter defining the shape of the distribution ($b = 0$ for isotropic distribution), μ is the main angle (it denotes the mean direction of fibres), ϕ is angle of an individual fibre and $I_0(b)$ is modified Bessel function of first kind of order zero.

Multimodal von Mises distribution was defined by (Masseran et al., 2013):

$$\rho_{mix}(\phi) = \sum_{i=1}^{N} \rho_i(\phi) = \sum_{i=1}^{N} \frac{1}{N \cdot \pi I_0(b_i)} \mathrm{e}^{b_i \cos(2\cdot(\phi-\mu_i))}, \quad (5)$$

where N is a number of modes (N=2 for bimodal, etc.), the meaning of the other parameters is same as for the unimodal distribution (4) but they differ for each mode.

Sometimes also different PDFs may be used; in (Schrauwen et al., 2012), PDF is used in the following form:

$$f_\alpha(\alpha, \alpha_1, \alpha_2, \sigma_1, \sigma_2) = A\left(\exp\left(\frac{\cos[2(\alpha-\alpha_1)]+1}{\sigma_1}\right) + \exp\left(\frac{\cos[2(\alpha-\alpha_2)]+1}{\sigma_2}\right)\right), \quad (6)$$

where α_1, α_2 are mean angles of fibre families, σ_1, σ_2 correspond to dispersion of fibres in these families, α is angle of an individual fibre and A stands as an normalizing factor.

3. Results

Since no paper published raw data, conversion of histograms into digital form was done using open source software (PlotDigitizer) as described in detail in (Fischer et al., 2019). The digitalized data were fitted with the respective PDF using Matlab's Curve Fitting Toolbox.

Data from (Schrauwen et al., 2012) were obtained for arterial adventitia under different inner pressure; comparison of their original bimodal and our unimodal approximation is shown in Tab. 2. However, since no qualitative measure of the fit was published there, we have calculated the values in Tab. 2 by fitting the data from (Schrauwen et al., 2012) using eq. (6). Both criteria show that in two of the evaluated cases the applied bimodal distribution is worse than the unimodal or isotropic (constant) distribution.

Tab. 2: Comparison between unimodal and bimodal distribution for Schrauwen et al., 2012.

Pressure [mmHg]	R^2/AIC bimodal (6)	R^2/AIC unimodal (4)	b (4)	μ [rad] (4)
0	**0.46/–359.48**	**0.84/–477.48**	1.05	–0.57
40	**–0.04/–397.85**	**0.00/–412.02**	–	–
80	0.74/–295.96	0.64/–268.43	1.92	1.20
120	0.91/–287.94	0.80/–269.56	2.63	1.39

(Jett et al., 2019) dealt with directions of collagen fibres in mitral valve leaflet under biaxial tension; they measured 4 states – unloaded tissue (A), two biaxial loadings (B, C) with 250 mN acting in one direction and 1000 mN in the other, and equibiaxial loading (D) with 1000 mN. The authors used the following modified von Mises distribution:

$$\rho(\theta|\mu_1, \kappa_1, \mu_2, \kappa_2, w) = w\rho_{vM}(\theta|\mu_1, \kappa_1) + (1-w)\rho_{vM}(\theta|\mu_2, \kappa_2), \quad (7)$$

where ρ_{vM} is unimodal von Mises distribution eq. (4), θ is a fibre angle measured from circumferential direction, $\mu_{1,2}$ are mean angles of fibre families, $\kappa_{1,2} \in [0, 1]$ are concentration parameters similar to b in eq. (4) and $w \in [0, 1]$ is mixing parameter. Two sets of measurement published there are compared in Tab. 3 and Tab. 4. Here the last column represents modified data with the isotropic part subtracted from the initial histogram and fitted by unimodal von Mises distribution. In some cases, it gave the goodness of fit comparable with the original bimodal distribution.

Tab. 3: Comparison of unimodal and bimodal distributions for the first data set in Jett et al., 2019.

Mode	R^2/AIC as published	R^2/AIC unimodal (4)	R^2/AIC bimodal (5)	R^2/AIC isotropic
A	$0.908/-254.87$	$0.55/-165.66$	$0.89/-246.20$	$0.86/-179.56$
B	**0.936/–274.84**	$0.67/-176.87$	$0.93/-266.03$	**0.92/–210.30**
C	$0.943/-303.32$	$0.43/-165.06$	$0.90/-266.13$	N./A.
D	**0.938/–273.74**	$0.77/-204.81$	$0.92/-263.58$	**0.86/–191.71**

Tab. 4: Comparison of unimodal and bimodal distributions for the second data set in Jett et al., 2019.

Mode	R^2/AIC as published	R^2/AIC unimodal (4)	R^2/AIC bimodal (5)	R^2/AIC isotropic
A	$0.875/-292.05$	$0.01/-176.97$	$0.87/-295.91$	N./A.
B	**0.903/–233.60**	$0.28/-112.48$	$0.91/-242.15$	**0.87/–150.29**
C	$0.813/-236.30$	$0.03/-136.79$	$0.82/-234.17$	N./A.
D	**0.971/–305.16**	$0.57/-150.40$	$0.97/-305.08$	**0.95/–220.54**

The last analysed study was (Schriefel et al., 2011) investigating three layers of thoracic (T) and abdominal (A) aorta and of common iliac artery (CI). The authors used 3D von Mises distribution but the histograms were published for one plane only, thus 2D von Mises distribution was used in this analysis (both unimodal and bimodal fits). As not all the histograms were published completely, only two layers of the wall (intima and media) were analysed. The results are presented in Tab. 5. In media – CI the unimodal and bimodal fits gave nearly the same quality.

Tab. 5: Comparison between unimodal and bimodal distribution for Schriefel et al., 2011.

Parameters	Unimodal fit				Bimodal fit					
	b	μ [°]	R^2	AIC	b_1	b_2	μ_1 [°]	μ_2 [°]	R^2	AIC
Intima – T	0.19	4.87	0.17	−307.56	1.29	1.31	50.69	−29.74	0.59	−351.33
Intima – A	0.42	9.49	**0.54**	**−154.34**	1.13	1.11	−21.1	40.19	**0.65**	**−158.72**
Intima – CI	0.09	−44.15	0.03	−180.71	1.02	1.31	46.1	−43.18	0.30	−191.09
Media – T	0.69	−5.76	0.51	−140.23	3.29	2.69	−26.6	23.80	0.95	−235.22
Media – A	0.94	2.79	0.68	−173.06	3.15	3.56	−30.4	19.83	0.95	−259.50
Media – CI	2.03	5.39	**0.92**	**−215.64**	2.03	3.94	21.46	−2.88	**0.93**	**−222.62**

4. Conclusions

The expected preference of Akaike information criterion was not confirmed, it never changed the preferred distribution based on the R^2 criterion as it happened in the fictitious illustrative example. On the other hand, it was shown by our analyses that the generally applied preference of bimodal distribution is disputable; unimodal distribution or its combination with a constant (isotropic distribution) was capable to give a better or comparable quality of the fit in some cases (highlighted in bold in all tables). Therefore, the quality of fit should be always evaluated and compared for different approximations of the obtained histograms and the best one should be chosen on the basis of some mathematical criterion, no matter which one.

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